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Coexisting superconducting and spiral spin order: models of ruthenate.

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Influence of a spiral spin structure on the superconducting (SC) pairing in the most probable active γ band of Sr_2RuO_4 is studied in the mean-field approximation. Such structure with "incommensurate" vector $Q = 2\pi(1/3, 1/3)$ has been proposed as that which removes the nesting instability in α, β bands. The pairing interaction of adjacent centers of two types - with attraction in singlet channel or in both the singlet and triplet channels - is adopted. In both cases the mixed singlet and triplet SC order is revealed. The d-wave singlet pairing is accompanied by formation of the p-wave triplet pairs $(k, -k-Q)_{\uparrow\uparrow}$ and $(k, -k+Q)_{\downarrow\downarrow}$ with large total momenta $\mp Q$ and spin projections ± 1 onto an axis normal to the spin rotation plane of the spiral structure. Both the superconducting and normal states have a broken time reversal symmetry which might be detected by polarised photoemission.

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I. INTRODUCTION

The problem of interplay between the superconducting and spin orders is actual for all compound with strong electronic correlations. Among them a single-layer quasi-2D ruthenate attracts considerable attention as a superconductor ($T_c \sim 1.5K$) with a possible triplet type of pairing [1,2]. One of the arguments in favor of such type of pairing is the Knight shift behavior [3]. It was suggested also that the pairing is governed by the ferromagnet (FM) fluctuations which certainly exist in the ferromagnetic parent compound $SrRuO_3$. The theoretical proposal [4,5] of a spin-triplet p-wave superconducting (SC) order parameter (OP) $\Delta_{ss'}(k) = (i\sigma_2\sigma_i)_{ss'}d_i(k)$ with $d_z(k) \sim k_x + ik_y$ is supported by the observed temperature independent Knight shift [3] and an increase of muon spin relaxation below T_c [6]. This OP corresponds to the nodeless gap function on the quasi-2D Fermi surface of Sr_2RuO_4. Similar nodeless solution is a natural choice in a weak-coupling theory [5]. However, the power temperature dependences as $T \to 0$, found for the specific heat, $C(T) \sim T^2$ [7], NQR relaxation rate, $T_1^{-1} \sim T^3$ [8], the thermal conductivity $\kappa(T) \sim T^2$ [9,10], the penetration depth [11], and ultrasonic attenuation [12] point to the node lines of the SC gap. In this connection the other possible gap symmetries have been discussed [13–16]. In particular, the f-wave symmetry gap function with a horizontal node plane have been proposed in [13]. It seems to support the observed 4-fold symmetry of anisotropic thermal conductivity of Sr_2RuO_4 under the in-plane magnetic field [9,10]. But the observed anisotropy is consistent also with a conventional d-wave pairing argued in some works. However, the latter hypothesis would require a new interpretation of the Knight shift behaviour.

The situation with both the SC order and the magnetic properties might be much more complicated if a normal state of the RuO_4 plane displays the spiral (static or dynamic) spin structure. The latter has been proposed recently [17] in order to describe the incommensurate peak in a spin susceptibility $\chi''(q, \omega)$ at $q \sim Q = 2\pi(1/3, 1/3)$ observed in inelastic neutron scattering [18,19] and some features in ARPES data [20] for Sr_2RuO_4. The properties of the quasi-1D sheets of Fermi surfaces (FS's) for the α and β valence bands at total occupancy 4 electron per site imply the nesting instability at $q = Q$ [21,22]. A spiral structure with $q = Q$ removes this instability

for both quasi-1D bands simultaneously even in zero order with respect to large on-centre interaction. In mean field approximation the energy of spiral state with $Q = q$ is really lower than that of the para-, ferro-, antiferromagnetic MF states [17]. The possibility of a coexistence of the SC pairing with a spiral order, as well as of the coexistence of an antiferromagnet (AF) and SC orders in cuprates, is yet an intriguing problem. It is interesting also since the spiral spin structure means a time-reversal symmetry breaking (TRSB) even in the normal state and a rich set of new mixed states with the coexisting singlet and triplet SC order parameters appear in the system. A new perspective of experimental study of TRSB phenomena has been open recently by an exciting results for the cuprates obtained with use of a photoemission (ARPES) with polarised photons [23].

The aim of present work is to study a possibility of coexistence of the spiral spin order and superconductivity in models having relation with Sr_2RuO_4. The symmetry and interplay of the singlet and triplet OP's are studied. It is shown that both types of pairs survive simultaneously in SC state in presence of spiral spin structure. It is confirmed that the most probable "active" band is the γ band. In this band the preferential singlet d-wave pairs coexists with the triplet pairs. Earlier [16] the possibility of mixing SC order in Sr_2RuO_4 has been supposed on base of very close condensation energies for states with different symmetries of pairing. It was considered that the pairing is mediated by spin supceptibility peaked at incommensurate momentum. Unlike [16] we derive a microscopic mixing of the d-wave singlet and p-wave triplet SC orders caused by the local spiral spin structure. The pairing is induced by model interaction of adjacent centres. First we test the models with the large pairing constants κ and corresponding large transition temperatures. Then we extend a study to more realistic models and calculate the phase curve $T_c(\kappa)$ in full range of pairing constant.

Preliminary several basic points of consideration must be outlined.

1.Since the SC pairing interaction is supposed to be of electronic nature, we try to model it by electronic interactions of adjacent sites of type

$$V = \sum_{<nm>,\nu} V_\nu n_{\nu n} n_{\nu m} + J_\nu \mathbf{S}_{\nu n} \mathbf{S}_{\nu m} \qquad (1)$$

for each of three bands $\nu = \alpha, \beta, \gamma$. This corresponds to taking into account the lowest k- harmonics in a momentum representation of pairing interaction $V_{kk'}$, like it has been done in [4]. Interaction (1) corresponds to the SC pairing constants $\kappa^s = 2V + J/2$, $\kappa^t = 2V - 3J/2$ in the singlet and triplet channels. The natural signs $V > 0$, $J > 0$ would be expected from an experience in field of strongly correlated systems. In the one-band models such signs of V, J correspond to $\kappa^t > 0$, $\kappa^s < 0$ in the triplet and singlet channels and thus they are more appropriate for a singlet, but not triplet pairing. Here we extend a study on the both signs of pairing constant κ^t in triplet channel.

2. The electronic structure of Sr_2RuO_4 is determined by three almost independent α, β, γ bands based on the d-orbits of Ru^{+2} of the $xz,\ yz,\ xy$ nature [21,22]. Only small hybridisation of xz and yz bands takes place at crossing points of their Fermi surfaces (FS's) at $k_x = \pm k_y$. According to [4,5] the orbital symmetry significantly suppresses also the interband Cooper pair scattering which induces the SC gap simultaneously in all sheets of FS's. So, a study is divided into the following stages. First one is a study of the SC pairing and its symmetry in each band separately and a selection of a most probable "active" band for SC instability. Then the interband scattering of Cooper pairs and the proximity effect [4] should be taken into account to provide a superconductivity in the whole three-band system. Here we concern only a first stage of problem.

3. In difference from [4] we start from the normal MF state with a broken time reversal symmetry, namely with a local spiral spin structure characterised by a diagonal vector $Q = 2\pi(1/3, 1/3)$. This is a normal state with the non-zero spin currents $j_\uparrow = -j_\downarrow$ of opposite directions for two different spin polarisations perpendicular to the spin rotation plane of the spiral state. This means that the electrons with up (down) polarisations occupy preferentially the k-states with $\mathbf{kQ} < 0$ or $\mathbf{kQ} > 0$ correspondingly. Such symmetry leads to the polarisation asymmetry of FS's revealed in [17] and it can lead also to formation of the mixed singlet and triplet pairing in

SC state of system.

II. MF TREATMENT IN A SPIRAL SPIN CONFIGURATION

A three-band model of RuO_4 plane is described by Hamiltonian [22]

$$H = T + H_U + V; \;\; T = \sum_{\nu,\sigma}\sum_{k} \epsilon_{\nu k} c^{\dagger}_{\nu k\sigma} c_{\nu k\sigma} \qquad (2)$$

$$H_U = \sum_{n,\nu}\Big\{ U n_{\nu n\uparrow} n_{\nu n\downarrow} + \sum_{\nu'\neq\nu} [U_2 \frac{1}{4} n_{\nu n} n_{\nu' n} - J \mathbf{S}_{\nu n}\mathbf{S}_{\nu' n}]\Big\}$$

Here $\nu = 1,2,3$ (or α,β,γ) correspond to bands of xz, yz, xy nature; $\epsilon_{\nu,k}$ and H_U are the zero band energies and the on-centre interactions with parameters from [22]. The interband interaction $T_{\alpha\beta} = \sum_{k,\sigma} 4t_{\alpha\beta}\sin k_x \sin k_y (c^{\dagger}_{1k\sigma} c_{2k\sigma} + h.c.)$ is small. So in normal state with any spin structure one have three almost independent bands with small mixing of the α,β bands at the crossing points of their FS's. We neglect this mixing. For a sake of simplicity we retain the notation α,β for the unmixed bands of xz, yz nature. Mutual influence of one band to other are provided by common chemical potential and by mean fields created by electrons of all bands. These fields are spin-dependent due to the on-centre exchange interaction. The interaction $V_{<nm>}$ of neighbour sites of type (1) is included in order to model the possible singlet and triplet pairing in system.

In MF approximation the energy averaged over an arbitrary BCS-like state is an explicit function

$$\overline{H} = \overline{H}^{N}(y_i) + \overline{H}^{SC}(w_j,\theta_j) \qquad (3)$$

depending on the normal (y_i) and anomalous (w_i,θ_j) one-electron averages named as OP's. Among the normal OP's $\{y_i\}$ there are the on-centre ($l=0$) and bond ($l = e_x, e_y$) densities $r^{\nu}(l) =< \frac{1}{2}\sum_{\sigma} c^{\dagger}_{n,\nu,\sigma} c_{n+l,\nu,\sigma} >$ in each band ν, the mean kinetic energies $T^{\nu}(l) =< \frac{1}{N}\sum_{k\sigma}\epsilon_k c^{\dagger}_{k\sigma} c_{k\sigma} >$ and the local ($l=0$) or bond ($l = e_x, e_y$) spin densities $\mathbf{d}^{\nu}(l)$. The local spin densities

$$d^{\nu}(0) = [d^{\nu}(0)]^{*} =< e^{iQn} c^{\dagger}_{n\nu\uparrow} c_{n\nu\downarrow} > \qquad (4)$$

determine the spiral spin structure with a spiral vector $Q = 2\pi(\frac{1}{3},\frac{1}{3})$

$$< \mathbf{S}_{n\sigma} >= \mathbf{e}_x \cos Qn + \mathbf{e}_y \sin Qn \qquad (5)$$

Previous calculations [17] show that the energy of normal spiral state with such Q is lower than the energies of the para-, ferro- and antiferromagnetic MF solutions. Such structure removes the nesting instability of the α,β bands and the exchange fields induce the same spiral spin structure in the γ band also. The MF solution gives the collinear contributions to the on-centre local spin from each band.

Since the FS's are different for all three bands, we should consider only the intraband anomalous averages determined by the large phase volume around the whole FS. A formation of pairs $(c^{\dagger}_{k\nu\uparrow} c^{\dagger}_{-k\nu'\downarrow})$ from different bands $\nu \neq \nu'$ would be effective only at small regions of k near the crossing points of their FS's. Contrary to such arguments recently [15] the interband pairing pairing mechanism has been proposed for Sr_2RuO_4. However, the comparative estimations of corresponding pairing susceptibility contradicts the possibility of such pairing. So we retain the intra-band SC OP's only and neglect the interband pair scattering. Then the expression for $\overline{H}^{SC}$ is

$$\begin{aligned} \tfrac{1}{N}\overline{H}^{SC} = \; & U|w_{\nu}(0)|^2 + \textstyle\sum_{\nu,\; l=e_x,e_y}\Big\{\kappa^{s}_{\nu}(l)|w_{\nu}(l)|^2 \\ & + \kappa^{t}_{\nu}(l)\textstyle\sum_{\mu=0,\pm1}\frac{1}{1+|\mu|}|\theta_{\mu,\nu}(l)|^2\Big\} \end{aligned} \qquad (6)$$

Here the quantities $w(l),\theta(l)$ are the singlet and triplet superconducting order parameters (SC OP's) on one centre ($l=0$) or on the neighbour centres ($l = e_x$ or e_y). They are determined as

$$w_{\nu}(l) = \frac{1}{2N}\sum_{n\sigma}\frac{\sigma}{|\sigma|} < c^{\dagger}_{\nu,n,\sigma} c^{\dagger}_{\nu,n+l,-\sigma} > \qquad (7)$$

$$\begin{aligned} \theta_{\nu\mu}(l) = \; & \tfrac{1}{2N}\textstyle\sum_{n\sigma} e^{i\mu Q(n+l/2)}(\sigma_{\mu}\sigma_{y})_{ss'} \\ & < c^{\dagger}_{\nu,n,s} c^{\dagger}_{\nu,n+l,s'} > \end{aligned} \qquad (8)$$

Here matrices σ_{μ} are σ_z or $\mp(\sigma_x \pm i\sigma_y)$ for $\mu = 0,\pm1$, and $\sigma_{x,y,z}$ are the Pauli matrices. The phases $\phi(n,l) = \mu Q(n+l/2)$ for $\mu = 0,\pm1$ in definition of the triplet OP's (8) provide that the contribution from each bond $< n, n+l >$ are independent on n in the same manner as the cyclic spin components $< S_{n\mu} e^{-i\mu Qn} >$ for $\mu = \pm1$ are independent on n for state with the spiral spin structure. These phases are connected with existence of the

spin currents in the spiral state. As it will be shown later the coupled triplet pairs ($\uparrow\uparrow$) or ($\downarrow\downarrow$) with the spins $\mu = 1$ or -1 occur to be a moving pairs carrying large total momenta $\pm Q$ correspondingly. The neighbour-centre pairing constants $\kappa^{s,t}$ in (6) are connected with the constants $V(l)$, $J(l)$ for the supposed interaction of type(1).

Having in mind an essential independence of α, β, γ bands, consider the possible SC orders in each band separately in order to study a symmetry of SC order compatible with the spiral spin order. Besides, we confirm the previous conclusion [4] that the most probable "active" band for SC instability is the γ band. In this line we neglect the interband Cooper pair scattering and take into account only the intra-band constants κ^s, κ^t in (7). To reduce the number of the SC OP's we use the arguments typical for all strongly correlated systems. At any interaction $V_{<nm>}$ in (1) a large on-centre interaction $U > 0$ suppresses the singlet s-wave pairing $w(0)$ in γ band according to Eq.(6). So we retain only the $d_{x^2-y^2}$-wave OP among the singlet OP's and take $w_\gamma(0) = 0$, $w_\gamma(e_x) = -w_\gamma(e_y)$. This provides the pair function which is orthogonal to the forbidden s-wave pair function. For quasi 1D α, β bands (here α, β refer to xz, yx bands rather than their combinations) the same on-centre interaction suppresses all singlet pairings and we put $w_{\alpha(\beta)}(0) = w_\alpha(e_x) = w_\beta(e_y) = 0$ since both combinations $w_\alpha(e_x) \pm w_\alpha(e_y)$ are non-orthogonal to the on-centre pair function $w(0)$ for the quasi- 1D bands with a broken tetragonal symmetry.

The neighbour site interaction of type (1) can induce the SC order only if some of the constants κ^s_ν, κ^t_ν in (6) are negative. Such "attraction" should be thought rather as that of a kinematic or correlational nature or due to the hybrid character of "site orbits" composed from the d- and p_π orbits of ruthenium and oxygen. For this reason we suppose that corresponding parameters $\kappa^s_\nu(l)$, $\kappa^t_\nu(l)$, or equivivalently $V_\nu(l)$, $J_\nu(l)$ in model interaction (1), have non-zero values only for those bonds $< nm >$, $m = n + l$, for which the hoping t^ν_{nm} is non-zero. This assumption is inspired by the expression for the exchange interaction $J_{nm} \sim 4t^2_{nm}/U$ in t-J model. So among all possible constants we set the non-zero values only for the following singlet (s) and triplet (t) pairing constants

$$\kappa^{s(t)}_\alpha(e_x) = \kappa^{s(t)}_\beta(e_y) = \kappa^{s(t)}_\gamma(e_x) = \kappa^{s(t)}_\gamma(e_y) = \kappa^{s(t)} \quad (9)$$

In the same analogy with t-J model one would expect the signs $\kappa^s = -\kappa^t < 0$. In connection with an expected triplet SC order in Sr_2RuO_4 [1] we especially extend our calculations on two limiting cases with both signs of the triplet constant

$$I.\ \ \kappa^s = -\kappa^t < 0; \qquad II.\ \ \kappa^s = \kappa^t < 0 \quad (10)$$

First case corresponds to an attraction of particles in the singlet channel, but repulsion in the triplet one. The second case corresponds to attraction in both channels.

The MF procedure is the standard one. From explicit function $\overline{H}(z_i)$ of mean energy depending on the one-particle OP's $z_j = \{y_i, w_i, \theta_i\}_j$ one obtains the linearised Hamiltonian

$$H_{Lin} - \mu N = \frac{\partial(\overline{H} - \mu\overline{N})}{\partial z_i}(\hat{z}_i - z_i) + \overline{H}(z_i) - \mu\overline{N} \quad (11)$$

where $\hat{z}_i$ are the one-particle operators corresponding to respective OP's z_i. The MF BCS-like state is the eigen state of H_{Lin} and in turn this state determines the values of OP's z_i. Thus the selfconsistent solution is obtained.

For the state with the spiral spin structure the most convenient basis set for representation of (11) is a basis of the following Fermi operators

$$b^\dagger_{i,\nu,k} = \left\{ c^\dagger_{\nu,k,\uparrow},\ c^\dagger_{\nu,k+Q,\downarrow},\ c_{\nu,-(k+Q),\uparrow},\ c_{\nu,-k,\downarrow} \right\}_i, \quad (12)$$

for each band ν. Here $i = 1, \ldots, 4$ and the momentum k runs inside the region F which is a half of whole momenta space and is limited by conditions

$$k \in F: \qquad (k + Q/2)Q < 0 \quad (13)$$

For vector Q with $Q_x = Q_y = 2\pi/3$ the Eq.(13) means that the components k_x, k_y vary in limits

$$-\pi - Q_x/2 < k_{x,y} < \pi - Q_x/2; \qquad k_x + k_y + Q_x < 0$$

The linearised Hamiltonian H_{Lin} is determined by the independent contributions in a basis subset (12)

$$H_{Lin} = \sum_{k \in F} \hat{h}^\nu_k; \qquad \hat{h}^\nu_k = h^\nu_{ij} b^\dagger_{i,\nu,k} b_{j\nu,k} \quad (14)$$

Here the fourth rank Hermitian matrix h^{ν}_{ij} is determined by elements (the omitted band index ν is implied here)

$$\begin{array}{ll} h_{11} = \epsilon_\nu(k_1) - \mu; & h_{22} = \epsilon_\nu(k_2) - \mu; \\ h_{12} = -h_{24} = -\frac{1}{2}\partial\overline{H}/\partial d_\nu; & h_{14} = A(k_1) + B_0(k_1); \\ h_{23} = -A(k_2) + B_0(k_2); & h_{13(2,4)} = B_{\pm 1}(\overline{k}); \\ h_{33} = -h_{22}; & h_{44} = -h_{11} \end{array} \quad (15)$$

where

$$k_1 = k, \quad k_2 = k + Q, \quad \overline{k} = (k_1 + k_2)/2$$

and the functions $A,\ B_\mu$ are

$$\begin{array}{ll} A(k) & = \sum_{l=e_x,e_y} \kappa^s_\nu(l) w_\nu(l) \cos kl; \\ B_\mu(k) & = \sum_{l=e_x,e_y} \kappa^t_\nu(l) \theta_{\mu,\nu}(l) \sin kl \end{array} \quad (16)$$

The d-wave symmetry of singlet OP in γ band requires the antisymmetry of $A^\gamma(k_x, k_y) = -A^\gamma(k_y, k_x)$ at $k_x \leftrightarrow k_y$. The MF solution reveals also the same values of θ_μ for $\mu = \pm 1$. So actually only three non-zero real order parameters determine all SC OP's in γ band. They are

$$z_i = (w_d,\ \theta_0,\ \theta_1)_i, \quad i = 1, 2, 3$$

$$\begin{array}{ll} w_d = & \frac{1}{2}[w(e_x) - w(e_y)],\ \theta_0 = \frac{1}{2}[\theta_0(e_x) - \theta_0(e_y)] \\ & \theta_1 = \frac{1}{4}\sum_{\mu=\pm 1}[\theta_\mu(e_x) - \theta_\mu(e_y)] \end{array} \quad (17)$$

The same symmetry with respect to $x \leftrightarrow y$ should be applied to the solutions in α, β bands, but with simultaneous replacement $\alpha \leftrightarrow \beta$ ($xz \leftrightarrow yz$). The same values of θ_μ for both projections $\mu = \pm 1$ are revealed in MF solution in $\alpha,\ \beta$ bands also. So, for α, β bands we retain the next triplet OP's corresponding to the non-zero triplet constants in (9):

$$\theta_{\mu,\alpha}(e_x) = -\theta_{\mu,\beta}(e_y); \quad |\mu| = 0,\ 1 \quad (18)$$

It was verified that if initial values of OP's satisfies Eqs.(17,18), then the subsequent iterations of selfconsisting MF procedure conserve the same symmetry.

One more simplification has been used. Really the interaction of type (1) gives the contribution to both parts $\overline{H}_N(y_i)$ and $\overline{H}_{SC}$ of the mean energy (3). We may consider that the first contribution depending on the normal state charge and spin densities is already taken into account in renormalised band energies $\epsilon_\nu(k)$ fitted earlier [22] to those obtained from the observed magnetic quantum oscillations. Thus we retain in $\overline{H}$ only the part of $< V >$ which depends on anomalous averages. The definitions (8) of the triplet OP's allows to deal with the real solutions. They have a certain symmetry relative to reflection in the diagonal plane $(z, x = y)$ containing the spirality vector Q with simultaneous exchange of bands $\alpha \leftrightarrow \beta$ and relative to reflection in plane $(z, x = -y)$ $(Q \to -Q)$ together with $\sigma \to -\sigma$.

The BCS-like spiral state under a search is determined by filling the one-particle eigen states $\chi^\dagger_{\lambda\nu k}$ corresponding the energy levels $E_\lambda(k)$

$$\chi^\dagger_{\lambda\nu k} = b^\dagger_{ik} S_{i\lambda}(k); \quad h_{ij}(k) S_{j\lambda}(k) = S_{i\lambda}(k) E_\lambda(k) \quad (19)$$

The matrices $S_{i\lambda}(k)$ of eigen-vectors and the Fermi occupancies $f(E_{\lambda\nu k})$ of levels determine the normal and anomalous OP's (7,8), thus closing the selfconsisting MF procedure.

III. THE RESULTS.

Since a full MF solution with SC order is easily obtained at large pairing constants, we first study the models with large $k^{s(t)}$. Then we present the phase curves $T_c(k^s)$ and relative values of SC OP's for realistic models with small k^s.

The results are obtained for two cases (10) of pairing constants corresponding to attraction in a singlet channel only (case I) or in both the singlet and triplet channels (case II). In first case the $\alpha,\ \ \beta$ bands do not display any own SC order. The reason is that both the singlet "d-wave", as well as "s-wave" OP are suppressed by on-centre interaction in bands with nonequivalent hopping in x and y direction: $t^\alpha_x \gg t^\alpha_y$ or $t^\beta_y \gg t^\beta_x$ (see parameters of three-band model in [22]). In difference, in γ band of system in spiral spin configuration the mixed SC order arises. The d-wave singlet order is accompanied by the triplet pair formation even at $\kappa^t_\gamma > 0$. Fig.1 shows the temperature dependence of the singlet and triplet OP's (17) of γ band for $\kappa^s = -\kappa^t = -0.6eV$. The value of triplet OP's occur to be $\theta_{+1,\gamma} = \theta_{-1,\gamma} \gg \theta_{0,\gamma}$. Taking into account the definition of the triplet OP's in (17,18) and their momentum representation one concludes that the coupled triplet pairs of particles of γ band

arise mainly in form ($\uparrow\uparrow$) or ($\downarrow\downarrow$) and these pairs are the moving coupled pairs carrying a large total momenta $-Q$ or Q correspondingly. This differs the triplet pairing in spiral state from that in isotropic Fermi liquid where only Cooper- like pairs $(k\uparrow, -k\uparrow)$ or $(k\downarrow, -k\downarrow)$ with zero momenta can exist. Moreover, unlike the isotropic model the triplet pairs arise even at positive value of triplet constant $\kappa^t > 0$ corresponding to repulsion in triplet channel.

Note that the emergence of coupled pairs with large total momentum $2k_F$ equal to a nesting vector was grounded in new theory of HTSC [24]. In [24] such pairs are the singlet pairs associated with the stripe structure. In case of the spiral state such moving pairs are the triplet ones. Note, that the photoemission technique with the circularly polarised photons recently applied to cuprates [23] could distinguish the supposed spiral structure which breaks a time reversal symmetry even in the normal state. In particular the sharp or smoothed (gaped) Fermi surfaces are predicted for electrons $(k\sigma)$ with momentum k from region $kQ < 0$ (or $kQ > 0$) and with polarisation $\sigma =\uparrow$ (or $\downarrow$) correspondingly. Really the spin order have a local finite-ranged character. Any disorder or any domain structure must suppress the above mention polarisation effects.

Thus an attraction only in a singlet channel leads to both the singlet and triplet pair formation in state with the spiral spin structure caused by nesting of α and β bands. Fig.1 shows also the heat capacity of system. A finite limit $C(T)/T$ at $T \to 0$ is due to contributions from α, β bands for which the normal state is retaining if the interband Cooper pair scattering is neglected.

Consider now the model of second type with "attraction" in both channels: $\kappa^s = \kappa^t < 0$ in (10) . At $\kappa^s > 0.65eV$ all three bands display their own SC order. At equal values of the pairing constants (9) in each bonds with large hopping the SC order in γ band has much pronounced character than that in α and β bands. The ensemble of coupled pairs in γ band consists mainly of the d-wave singlet Cooper pairs $\{k\uparrow, -k\downarrow\}^s$ and the moving triplet pairs $\{k\uparrow, -(k+Q)\uparrow\}$ or $\{k\downarrow, -(k-Q)\downarrow\}$ with total momentum $-Q$ or Q correspondingly. In α, β bands the triplet order is providing mainly by a Cooper-like triplet pairs $\{k\uparrow, -k\downarrow\}^t$ with a zero total momentum. They correspond to $\theta_0^\alpha(e_x) = -\theta_0^\beta(e_y) \neq 0$. Fig. 2 illustrates the temperature dependence of the SC OP's in α, β, γ bands at large trial constants $\kappa^s = \kappa^t = -0.8$eV. Note, that a relation $|\theta_0(l)| > |\theta_{\pm1}(l)|$ of triplet components for $l = e_{x(y)}$ in $\alpha(\beta)$ band differs from a relation $|\theta_0(l)| \ll |\theta_{\pm1}(l)|$ for γ band. This is connected with a difference in the Fermi surfaces and in the angular dependence of pairing potentials. Thus, our calculations confirm the conclusion [4] that the active band in system is the γ band. The independent SC transitions in different bands are accompanied by two steps in the temperature dependence of a heat capacity. It is seen that $C(T)/T \to 0$ at $T \to 0$ as it must be for the totally SC state. But since the scales of the SC OP's are different for γ and α, β bands a decrease of $C(T)/T$ at $T \to 0$ occurs at small T. Real situation should greatly depend on the inter-band pair scattering neglected here.

The pairing potential in active γ band with the SC OP's (17) may be presented in form

$$\begin{array}{l} H_{Lin}^{SC} = \sum_{k\in G}\{[A(k) + B_0(k)]c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger + B_1(k)\times \\ [c_{k-Q/2,\uparrow}^\dagger c_{-k-Q/2,\uparrow}^\dagger + c_{k+Q/2,\downarrow}^\dagger c_{-k+Q/2,\downarrow}^\dagger] + h.c.\} \end{array} \quad (20)$$

Here k runs the whole phase space G (in difference from representation (14), where k runs only half of G) and the omitted index $\nu = \gamma$ is implied. Functions $A(k)$, $B_\mu(k)$ are defined by Eqs.(16,17) and have a form

$$\begin{array}{ll} A(k) = & \kappa^s w_d(\cos k_x - \cos k_y); \\ B_\mu(k) = & \kappa^t \theta_\mu(\sin k_x - sin k_y) \end{array} \quad (21)$$

They obey the symmetry $A(k_x, k_y) = -A(k_y, k_x)$ and $B(k_x, k_y) = -B(k_y, k_x)$. Therefore in any cases the diagonal line $k_x = k_y$ along the vector Q is the node line of the gap function in our solution. Thus, in spiral state both the d-wave singlet and p-wave triplet SC orders are compatible. In case of isotropic normal state without the spiral spin structure ($d_\nu = 0$, $Q = 0$) the pairing potential (21) would be a superposition of contributions corresponding to different representations of tetragonal point group classified in [5]. In notations [5] this superposition may schematically be presented as $\{\theta_1(A_{1u} - B_{1u} - A_{2u} + B_{2u}) + \theta_0(E_{ux} - E_{uy})\}$. In difference from paramagnet state in spiral state the coupled pairs ($\uparrow\uparrow$), ($\downarrow\downarrow$) are the pairs with large total momentum

$\mp Q$. The spin currents $j_{\uparrow\uparrow} = -j_{\downarrow\downarrow}$ due to the pair motions are of the same signs as the spin currents $j_\uparrow = -j_\downarrow$ in the normal state with the spiral structure. Remind, that the spins are projected on the axis z perpendicular to the spin rotation plane of the spiral ground state structure (5).

The gap function in the γ band corresponding the paring potential (21) can be defined as a real matrix element

$$G(k) =< \eta_{-k}|H^{SC}|\eta_k^\dagger > \qquad (22)$$

between the electron and hole quasiparticles $\eta^\dagger, \eta$ of the upper Hubbard band of the normal spiral state.

Fig. 3 present the map of levels of the gap function $G(k)$ of γ band for case $\kappa^s = -k^t < 0$. The gap function is antisymmetric relative to an exchange $k_x \to k_y$ but does not possess the inversion symmetry. However, an imagine photoemission experiment for the γ band could measure two different gaps $|G(k)|$ and $|G(-k)|$ at each k for different polarisations (up and down) of the emitted electrons. Note, that along the known FS of γ band the function $G(k)$ is close to the d-wave function $\sim \cos k_x - \cos k_y$. This is consistent with the observed 4-fold anysotropy of heat conductance in the in-plane magnetic field [9,10].

Up to now the results refer to models with too large pairing constants and T_c. For more realistic models with small T_c and the pairing constants of both types (10) we carry out the calculations of the phase curves $T_c(\kappa^s)$. Dependence $T_c(\kappa^s)$ of the SC transition temperature in γ band is determined by equation following from linear expansion of r.h.s. of (7,8) over $w_\gamma, \theta_{\gamma\mu}$

$$Det \parallel \delta_{ij} - R_{ij}\kappa_j \parallel = 0 \qquad (23)$$

Here i, j numerate the SC OP's $\{z_i\}$ and a matrix R_{ij} is

$$R_{ij} = \frac{1}{N}\sum_k \sum_{\lambda,\lambda'} M^i_{\lambda,\lambda'} M^j_{\lambda,\lambda'} \frac{f(-E_\lambda) - f(E_{\lambda'})}{E_\lambda + E_{\lambda'}} \qquad (24)$$

where $E_\lambda, f(E_\lambda)$ are the normal state energies and the Fermi occupancies. Matrices M^i, $i = 1, 2, 3$, corresponding to SC OP's (17) are given in Appendix and constants κ_j in (23) are $\kappa_j = \{\kappa^s, \kappa^t, \kappa^t\}_j$. The indices $\lambda, \lambda' = 1, 2$ numerates the normal state levels in the upper and lower subband of γ band. At the transition points $T = T_c$, when Eq.(23) is satisfied, the corresponding homogeneous equations

$$(\delta_{ij} - R_{ij}\kappa_j)\tilde{z}_j = 0; \quad \tilde{z}_j = z_j^\gamma / \sqrt{z_1^2 + z_2^2 + z_3^2} \qquad (25)$$

determine the relative normalised values $\tilde{z}_j$ of the SC OP's. Fig. 4 presents the phase curves $T_c(\kappa^s)$ and relative values of OP's $\tilde{z}_j$ at $T \to T_c$ as function of κ^s for two signs of triplet pairing constant κ^t in (10). Points mark the values $\tilde{z}_j$ for $T \sim 0.6T_c$ obtained from full MF calculations for the above studied models. These values are in consistency with those obtained from Eqs.(25). The models with a realistic small $T_c \sim 10^{-4}$eV display the same symmetry properties of SC state as the models with large κ^s and T_c. The transition temperature $T_c = 1.5K$ observed in Sr_2RuO_4 corresponds to values $\kappa^s = 0.145\ eV$ or $\kappa^s = 0.12\ eV$ for each types (10) of models.

Many important problems concerning Sr_2RuO_4 remain out of the present study, for example a proximity effect, i.e. a mutual influence of different bands via the interband pair scattering [4]. This effect should be included in order to describe the observed common SC transition in all three bands. Its relation to the thermodynamics and magnetic properties have been discussed intensively [4,15,17].

IV. CONCLUSIONS

The above model treatment leads to following conclusions. The SC pairing in γ band can coexist with a spiral spin order caused by the nesting in α, β bands of Sr_2RuO_4. The most probable "active" band relative to the SC instability is the γ band. The mixed d-wave singlet and p-wave triplet SC order arises from the pairing interaction of adjacent sites on background of the normal state with the spiral spin structure described by the nesting vector $Q = 2\pi(1/3, 1/3)$. For both types of pairing constants - with attraction in the singlet and triplet channels or only in the singlet one - the main coupled pairs in system are the singlet d-wave pairs $(k, -k)^s_{\uparrow\downarrow}$ and the moving triplet pairs $(k - Q/2, -k - Q/2)^s_{\uparrow\uparrow}$, $(k + Q/2, -k + Q/2)^s_{\downarrow\downarrow}$ with large total momenta $\mp Q$ and with the spin projections $\mu = \pm 1$ on an axis normal to

the spin-rotation plane of the spiral structure. The preferential d-wave pairing in γ band is consistent with the observed 4-fold anysotropy of heat conductance in the in-plane magnetic field [9,10]. Only triplet SC order may be transfered from γ to α, β bands via interband pair scattering. The studied spiral normal and SC states are both the states with a broken time reversal symmetry. The effects of symmetry breaking might be detected in photoemission with circularly polarised light. The important questions remain unsolved: Can the mixed singlet-triplet pairing induced by attraction in singlet channel provide an independency of the Knight shift on temperature at $T < T_c$? Can the other periodic structures (besides the spiral one) exist in the normal state of Sr_2RuO_4 and what is a relation between the triplet and singlet SC pairing in these structures?

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V. APPENDIX

The matrices M^i in (24) are given by

$$M^i_{\lambda,\lambda'}(k) = \left[\begin{pmatrix} c & s \\ s & -c \end{pmatrix} \overline{M}^i \begin{pmatrix} s & c \\ c & -s \end{pmatrix} \right]_{\lambda\lambda'} \tag{26}$$

$$\overline{M}^1 = \begin{pmatrix} 0 & c_d(k_1) \\ -c_d(k_2) & 0 \end{pmatrix}, \quad \overline{M}^2 = \begin{pmatrix} 0 & s_p(k_1) \\ s_p(k_2) & 0 \end{pmatrix},$$
$$\overline{M}^3 = s_p(\overline{k}) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Here $s = \sin\varphi$, $c = \cos\varphi$ and $\varphi(k)$ for band ν is determined by equation $\tan(2\varphi) = -[\partial\overline{H}/\partial d_\nu][\epsilon(k_1 - \epsilon(k_2)]^{-1}$. The other functions are $c_d(k) = (\cos k_x - \cos k_y)/2$, $s_p(k) = (\sin k_x - \sin k_y)/2$ and $k_1 = k$, $k_2 = k + Q$, $\overline{k} = k + Q/2$.

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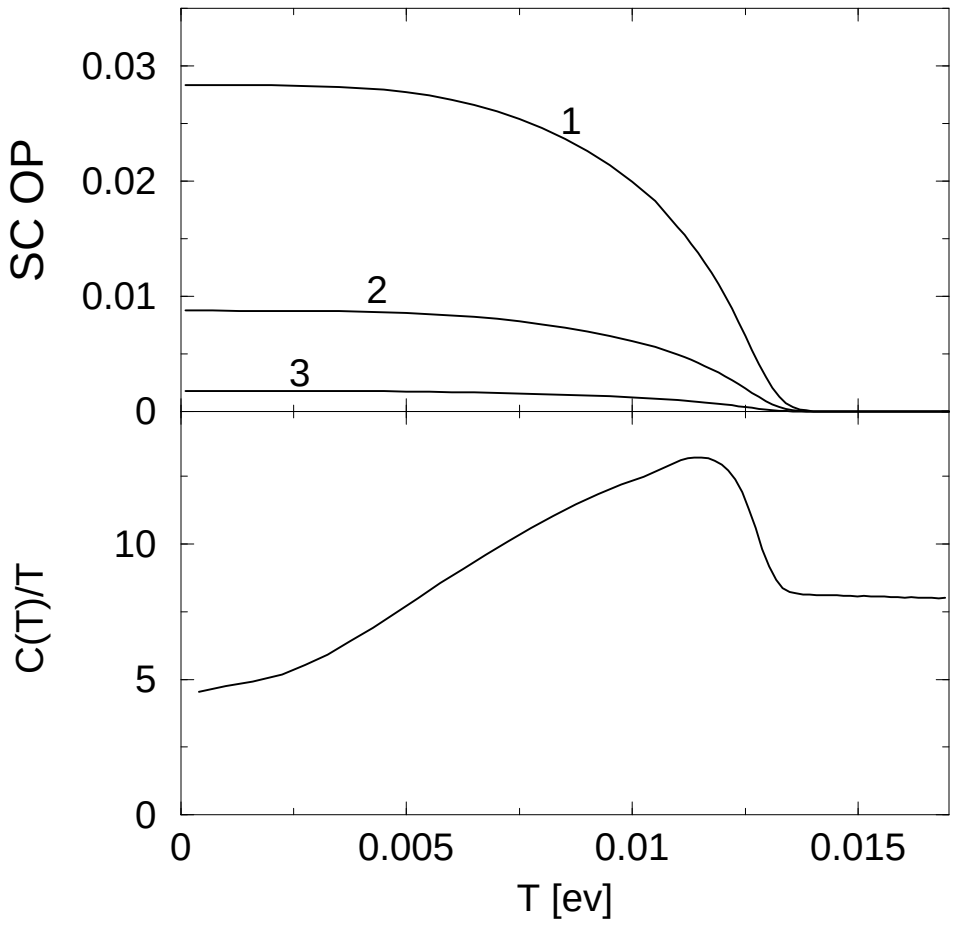
Captions to Figures

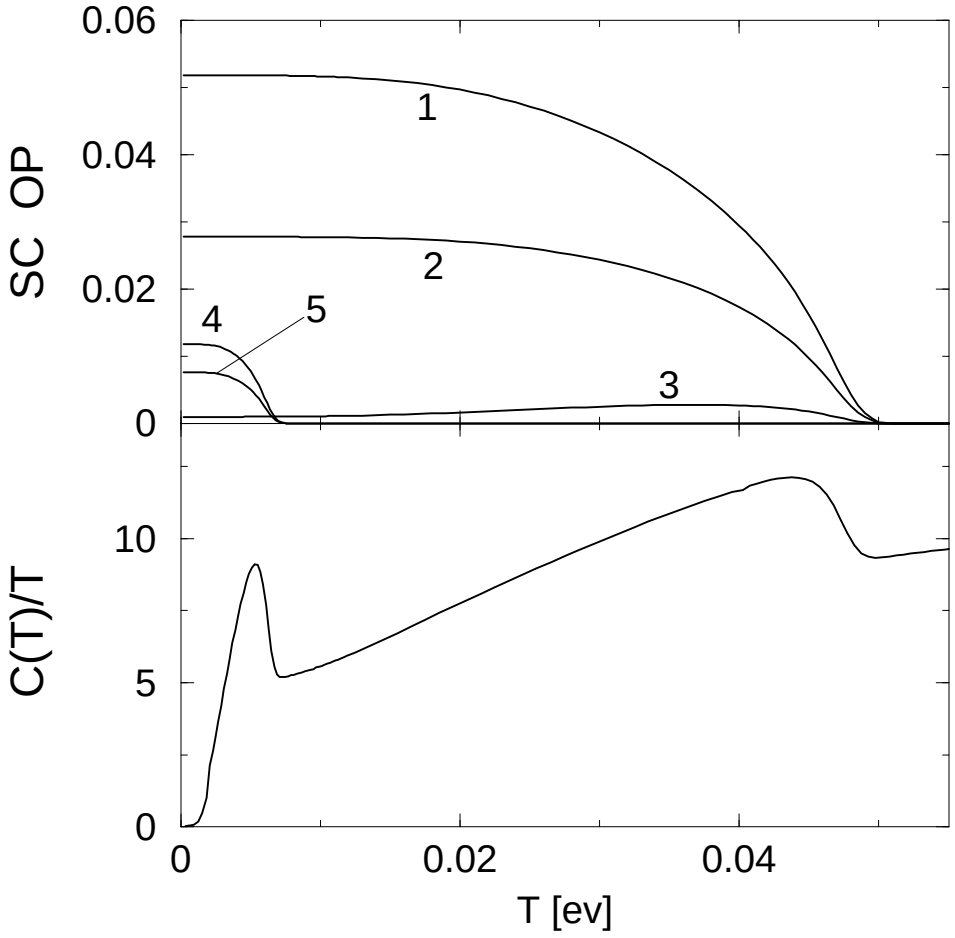
FIG. 1. The total heat capacity devided by T - $C(T)/T$ (in $[eV^{-1}]$) and the SC OP's in γ band as functions of temperature for model with independent bands and large pairing constants $\kappa^s = -\kappa^t = -0.6eV$. Curves 1-3 refer to w_d, $-\theta_0$ and $-\theta$ determined by Eq.(17).

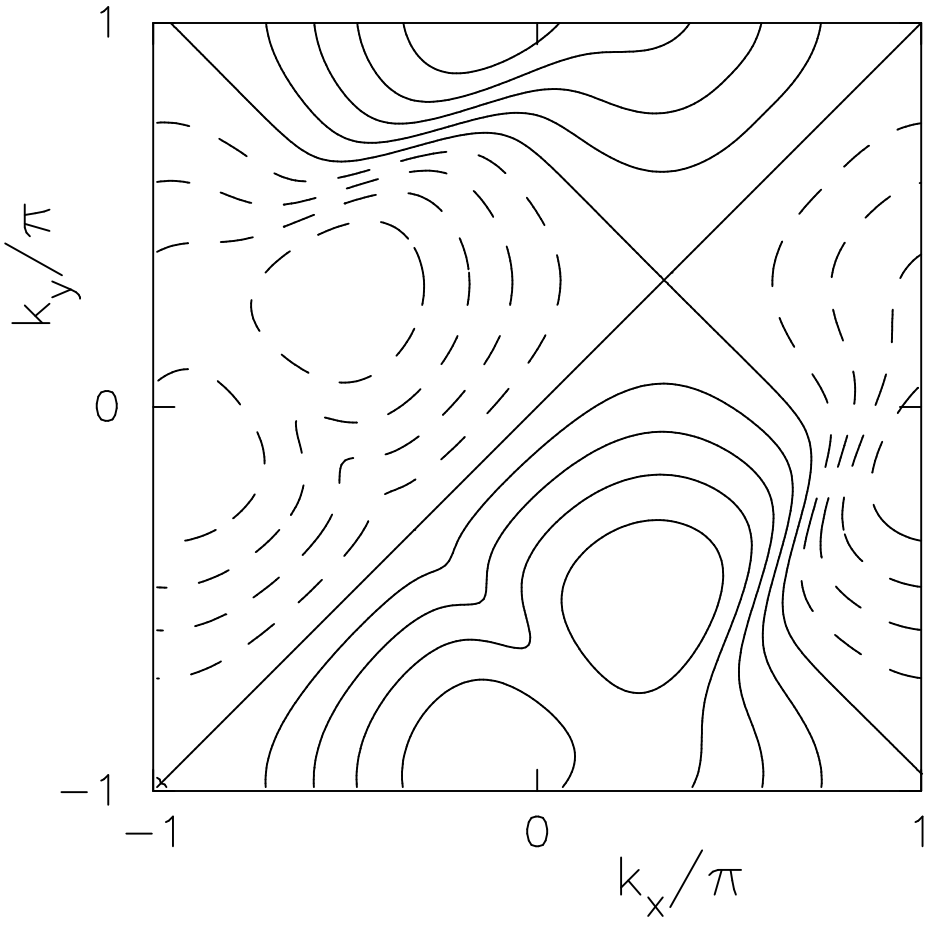
FIG. 2. The same as in Fig. 1 for model with $\kappa^s = \kappa^t = -0.8eV$. Curves 1-3 refer to the same OP's of γ band as in Fig. 1, curves 4,5 refer to $\theta_0^\alpha(e_x) = -\theta_0^\beta(e_y)$ and $\theta_{\pm 1}^\alpha(e_x) = -\theta_{\pm 1}^\beta(e_y)$.

FIG. 3. The contour map of the gap function (23) for the same model as in Fig. 1 in a momentum space $|k_{x(y)}| < \pi$. Solid (dashed) levels refer to positive (negative) values of gap function $G(k_x, k_y)$.

FIG. 4. Phase curves $T_c(\kappa^s)$ and the relative normalised values of OP's (25,17) of γ band as functions of the singlet pairing constant. Solid (dashed) curves refer to models with $\kappa^t = \pm\kappa^s$ correspondingly. Curves 1,2,3 refer to $\tilde{z}_i$, $i = 1, 2, 3$, obtained from solution of homogeneous equations (27) ($T \to T_c$). Points (circles and squares) are the same values at $T = 0.6T_c$ obtained from full MF calculations for the the models which are presented in Fig. 1 and Fig. 2 correspondingly.


SC OP
0.03
0.02
0.01
0
1
2
3
C(T)/T
10
5
0
0
0.005
0.01
0.015
T [ev]


0.06
0.04
0.02
0
SC OP
1
2
3
4
5
10
5
0
C(T)/T
0
0.02
0.04
T [ev]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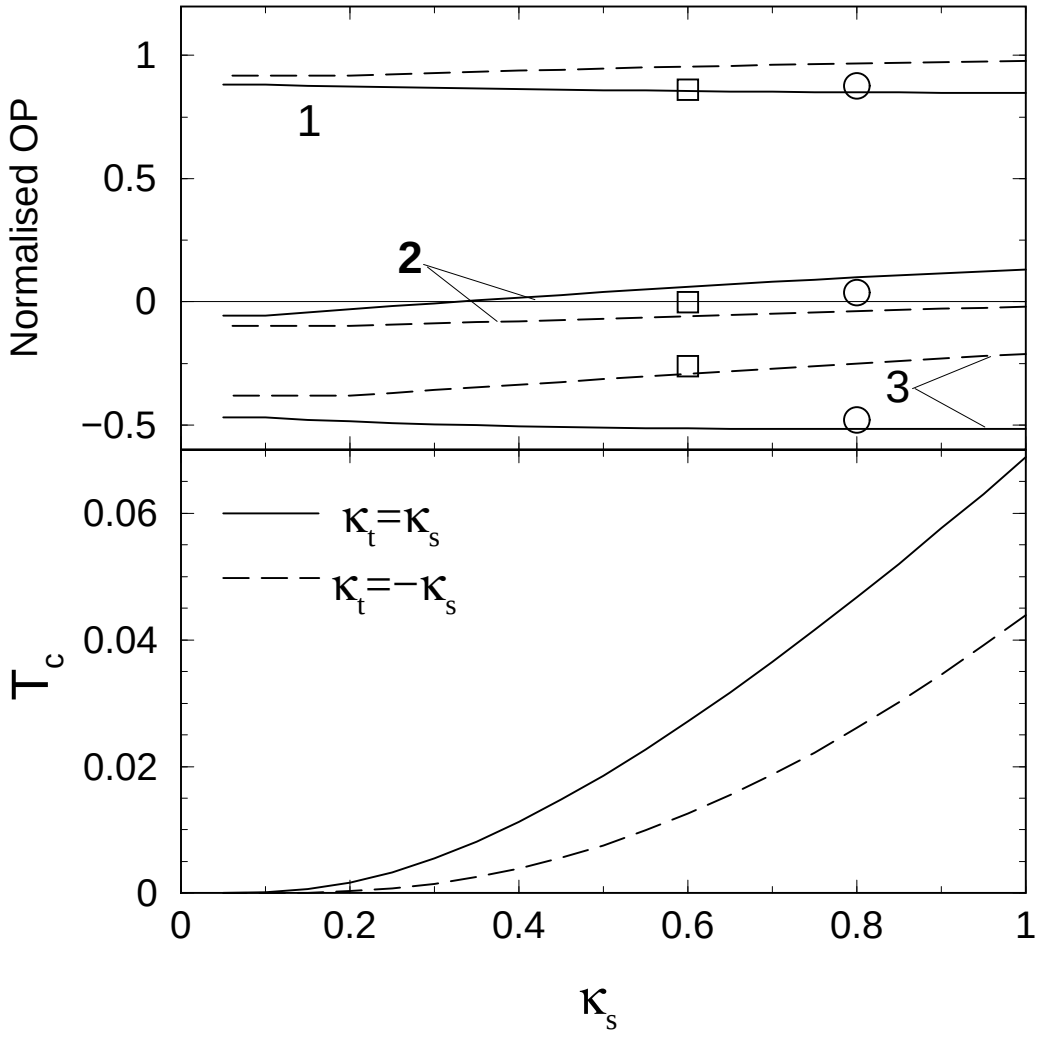
k_y/π
−1
0
1
k_x/π


Normalised OP
1
0.5
0
−0.5
1
2
3
T_c
0.06
0.04
0.02
0
$\kappa_t=\kappa_s$
$\kappa_t=-\kappa_s$
0
0.2
0.4
0.6
0.8
1
κ_s